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Abstract. In this paper we work on the estimation of a regression function that belongs to a polynomial eigenvalue decay reproducing kernel Hilbert space (RKHS). We describe the spectral filter framework for our estimator that allows us to deal with several iterative algorithms: gradient descent, Tikhonov regularization, etc. The main goal of the paper is to propose a new early stopping rule by introducing the smoothing parameter for the empirical risk of the estimator in order to improve the previous results [1] on the discrepancy principle. Theoretical justifications as well as simulations experiments for the proposed rule are provided.

Keywords. Non-parametric regression, regularization, kernels, stopping rules.

Résumé. Dans ce travail, nous présentons, dans un cadre général, l'estimation de la fonction de régression lorsqu'elle appartient à un RKHS. Les propriétés de plusieurs estimateurs sont analysées à travers des algorithmes itératifs comme la descente de gradient et la régularisation de type Tikhonov. L'objectif principal de notre analyse est de proposer une nouvelle règle d'arrêt prématuré des algorithmes basée sur l'introduction d'un paramètre de lissage dans la définition du risque empirique. Nous illustrons l'efficacité de notre approche et présentons les résultats d'une étude de simulation.

Mots-clés. Régression non-paramétrique, régularisation, noyaux, règles d'arrêt

1 Introduction

In supervised learning, given a sample of pairs of inputs and outputs, the goal is to estimate a regression function in the framework of empirical risk minimization or Tikhonov regularization. Usually properties of the regression function is not known, therefore one can apply different nonparametric techniques to relax this difficulty. Kernel methods [2] are one of the most widely used approaches to learning.

Early stopping rule (ESR) is an algorithmic approach to the regularization of an iterative algorithm such as (stochastic) gradient descent [3], boosting algorithms [4] or EM algorithm [5]. It is based on the idea of stopping an iterative process according to a special criterion in order to reach the best statistical precision. ESR has a fairly long history and was first introduced for artificial neural networks [6].

There have been three principal strategies for designing an ESR for a regression function learning. The first one is based on expanding the value of the risk error into the Taylor series and optimizing each term of the series. The second one consists in decomposing the risk error into the bias and variance parts, and in obtaining their high probability upper bounds. At the end, the stopping rule will be defined according to a criterion of the intersection of these two bounds. Several results have been derived regarding this strategy to quantify the ESR performance in the reproducing kernel Hilbert space (RKHS). For example, [7] derived a stopping rule when the regression function belongs to RKHS $\mathcal{H}$. If one stops the learning process at this iteration, the minimax optimal rate for the risk error is achieved for a wide class of functions. The main deficiency of this method is that it requires an accurate upper bound on the $\mathcal{H}$-norm of the regression function. The third and the recent one strategy consists in designing an ESR by observing the empirical risk and building a threshold for stopping appropriately an iterative process

(the so-called discrepancy principle). This approach was developed initially by [1], where the authors analyzed the behaviour of the discrepancy principle for spectral filter algorithms in the linear regression model that was further expanded to the kernel framework.

In the present work we keep the same spectral framework as in [1], by considering gradient descent and kernel ridge regression (or Tikhonov regularization) algorithms. More precisely, we focus on the nonlinear regression function estimation using the polynomial eigenvalue decay reproducing kernels. We introduce a smoothing parameter for the empirical risk, modify the previously designed discrepancy principle rule and prove an optimality result in terms of the $L_2(\mathbb{P}_X)$ out-of-sample error for the regression function estimator stopped at the new rule.

The organization of the paper is as follows. Section 2 introduces the statistical framework and the spectral filter estimator. Section 3 describes the main theoretical result achieved. Section 4 shows the behaviour of the derived ESR in simulations.

2 Statistical framework

Let us assume that we have a sample $z_i = (x_i, Y_i) \sim \mathbb{P},\ i = 1, ..., n$, with $x_i \in \mathcal{X}$ and $Y_i \in \mathbb{R}$, and we consider the usual regression model:

$$Y_i = f^*(x_i) + \sigma\epsilon_i, \quad i = 1, ..., n,$$

where ϵ_i are i.i.d. $\mathcal{N}(0, 1)$ random variables, $\sigma = \text{const}$ is known. Notice that there is a large body of work on estimating the noise variance σ^2 in the non-parametric regression. In other words,

$$Y = [Y_1, \ldots, Y_n]^\top = F^* + \sigma\epsilon \in \mathbb{R}^n.$$

Let us introduce now $(\hat{\mu}_1, \ldots, \hat{\mu}_n)$ and $(\hat{u}_1, \ldots, \hat{u}_n)$ as the eigenvalues and eigenvectors of the normalized Gram matrix $K = \mathbb{K}(x_i, x_j)/n$ respectively, where $\mathbb{K}(\cdot, \cdot)$ denotes the reproducing kernel associated with the reproducing kernel Hilbert space $\mathcal{H}$ [8]. Further, assume that

$$\hat{\mu}_1 \geq \hat{\mu}_2 \geq \ldots \geq \hat{\mu}_r > 0 = \hat{\mu}_{r+1} = \hat{\mu}_{r+2} = \ldots = \hat{\mu}_n.$$

We consider a mild assumption that $f^* \in \mathcal{H}$, and we would like to use an iterative learning algorithm to solve

$$\inf_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} (Y_i - f(x_i))^2 \right\} = \min_{\theta \in \mathbb{R}^n} \|Y - K\theta\|_n^2, \tag{1}$$

by the representer theorem [8]. Then, projecting $F^t = K\theta^t$, F^* , Y and ϵ onto the space spanned by $(\hat{u}_1, \ldots, \hat{u}_r)$, the r first eigenvectors of K, gives us

$$Z_i = G_i^* + \sigma\tilde{\epsilon}_i, \quad i = 1, \ldots, r.$$

Here, we used the fact that $G_i^* = \langle F^*, u_i \rangle = 0$ when $i > r$, since $f^* \in \mathcal{H}$.

A non-negative function $\gamma^{(t)} \in \mathbb{R}^n$ is called a spectral filter if it is a non-decreasing function of t (in each of its coordinates), $\gamma_i^{(0)} = 0$ and $\lim_{t\to\infty} \gamma_i^{(t)} = 1,\ i = 1, \ldots, r$. Several iterative algorithms could be expressed in terms of spectral filter as

$$(G^t)_i = \begin{cases} \gamma_i^{(t)} Z_i, & \text{if } i = 1, \ldots, r, \\ 0, & \text{if } i = r+1, \ldots, n. \end{cases}$$

Two examples that we study in this paper:

- Gradient descent (GD) with a constant step-size α: $\gamma_i^{(t)} = 1 - (1 - \alpha\hat{\mu}_i)^t$.
- (Iterative) kernel ridge regression (KRR) with a parameter α: $\gamma_i^{(t)} = \frac{\hat{\mu}_i}{\hat{\mu}_i + \lambda_t}$, where $\lambda_t = 1/(\alpha t)$ for the linear parameterization case or $\lambda_t = 1/(e^{\alpha t} - 1)$ for the exponential parameterization case.

3 Main results

3.1 Previous stopping rule definition

Considering the risk of the estimator F^t, we can define its bias and variance:

$$\mathbb{E}_\epsilon ||F^t - F^*||_n^2 = ||\mathbb{E}_\epsilon F^t - F^*||_n^2 + \mathbb{E}_\epsilon ||F^t - \mathbb{E}_\epsilon F_t||_n^2 = B_t^2 + \mathbb{E}_\epsilon V_t,$$
$$B_t^2 = \frac{1}{n}\sum_{i=1}^{n}(1 - \gamma_i^{(t)})^2 (G_i^*)^2, \quad \mathbb{E}_\epsilon V_t = \frac{\sigma^2}{n}\sum_{i=1}^{r}(\gamma_i^{(t)})^2.$$

Bias is a non-increasing convex functions converging to zero and variance is a non-decreasing function converging to $\frac{r\sigma^2}{n}$. Ideally we would like to be able to minimize the risk as a function of t. Actually, this is not possible because it depends on the unknown distribution $\mathbb{P}$. To overcome this problem, we define the empirical risk, a non-increasing convex function converging to zero.

$$R_t = \frac{1}{n}||F^t - Y||_2^2 = \frac{1}{n}\sum_{i=1}^{n}(1 - \gamma_i^{(t)})^2 Z_i^2.$$

A stopping rule that was designed in [1] consists in properly setting a threshold for the empirical risk:

$$\tau = \inf\left\{t > 0 : R_t \leq \sigma^2\right\}. \tag{2}$$

The following theorem describes the performance of τ compared to the optimal performance.

Theorem 3.1 (Oracle-type inequality) *For the gradient descent and kernel ridge regression filters, there exist constants $C_1 \geq 2$ and $C_2 > 0$:*

$$\mathbb{E}_\epsilon ||F^\tau - F^*||_n^2 \leq C_1 \mathbb{E}_\epsilon ||F^{t^*} - F^*||_n^2 + C_2 \frac{\sqrt{r}}{n},$$

where $t^* = \inf\left\{t > 0 : \mathbb{E}_\epsilon R_t \leq \sigma^2\right\}$.

Here, constants C_1 and C_2 do not depend on the number of samples n. This theorem shows that, if our kernel is a finite-rank one, then the remainder term is of the order $\mathcal{O}(\frac{\sqrt{r}}{n})$ and it is converging faster that the optimal value of the risk error, which is of the order $\mathcal{O}(r/n)$ [7]. However, if we assume that the rank of the kernel depends on the number of samples, e.g. for the Sobolev kernel, then the remainder term of the oracle-type inequality has a slow convergence rate (for the Sobolev kernel it is of the order $\mathcal{O}\left(\frac{1}{\sqrt{n}}\right)$). Moreover, it appeared that τ, since it is a random quantity itself, has a large variance. Therefore, we suggest using a smoothed version of the bias/variance and empirical risk by means of the eigenvalues of the Gram matrix, and a smoothing parameter $\theta \in [0, 1]$:

$$B_{\theta,t} = \frac{1}{n}\sum_{i=1}^{r}\hat{\mu}_i^\theta (1 - \gamma_i^{(t)})^2 (G_i^*)^2, \quad \mathbb{E}_\epsilon V_{\theta,t} = \frac{\sigma^2}{n}\sum_{i=1}^{r}\hat{\mu}_i^\theta (\gamma_i^{(t)})^2,$$
$$R_{\theta,t} = \frac{1}{n}\sum_{i=1}^{r}\hat{\mu}_i^\theta (1 - \gamma_i^{(t)})^2 Z_i^2, \quad \theta \in [0, 1].$$

3.2 Polynomial decay kernels

Let us, at the beginning, derive a result that introduces the minimax optimal rate for a stopping rule that has a $\mathcal{O}\left(\frac{1}{n}\right)$ threshold for the smoothed empirical risk, with the polynomial eigenvalue decay kernels.

Theorem 3.2 (Out-of-sample rate) *For any $\gamma > 0$ and $n \geq 16$, assume that $(x_1, \ldots, x_n) \sim \mathbb{P}_X$, and let us make the following assumptions:*

- $\sup_{x \in \mathcal{X}} \mathbb{K}(x, x) \leq M_K$.
- $|Y_i| \leq M$ *a.s. for any* $i \in \{1, \ldots, n\}$.
- *Let us define the kernel integral operator*

$$B : L_2(\mathbb{P}_X) \to L_2(\mathbb{P}_X),\ g \mapsto \int \mathbb{K}(\cdot, x) g(x) d\mathbb{P}_X(x).$$

  There exists $w \in L_2(\mathbb{P}_X)$ such that $f^* = B^{\nu - \frac{1}{2}} w$, with $\|w\|_{L_2(\mathbb{P}_X)} \leq M_K^{-\nu} \rho$ and $\nu \geq \frac{1}{2}$.

- *Given two parameters $s \in (0, 1)$ and $D \geq 1$, we consider the polynomial effective dimensionality*

$$\mathcal{N}(\lambda) = Tr(B(B + \lambda I)^{-1}) \leq D^2 (M_K^{-1} \lambda)^{-s}.$$

  This notion was first introduced by [9] in a learning context, and used in a number of works since. This assumption is tightly connected with the decay of the eigenvalues of the kernel integral operator B: if the eigenvalues of the kernel integral operator has a decay $\mu_i \asymp i^{-\frac{1}{s}}$, then the mentioned condition on the effective dimensionality holds true with the parameter s.

- *If we define an ESR $\hat{t}_o = \inf \left\{ t > 0 : R_{\theta,t} \leq C(\rho, D, M, M_K, \nu, \theta, \gamma)\ n^{\frac{2\nu+\theta}{2\nu+s}} \right\}$ for the gradient descent and kernel ridge regression filters, and we take the smoothing parameter $\theta = s$, then*

$$\|f^{\hat{t}_o} - f^*\|_{L_2(\mathbb{P}_X)} \lesssim n^{-\frac{\nu}{2\nu+s}} \text{ with probability } 1 - \gamma.$$

The rate achieved for the $L_2(\mathbb{P}_X)$-error in the theorem is proved to be minimax-optimal (see, e.g. [10])

The theorem shows that, if we choose the smoothing parameter $\theta = s$, our stopping rule strategy $\hat{t}_o$ will be optimal in the minimax sense. Since in practice we do not have an access to the eigenvalues of the kernel integral operator, we propose using the inverse decay of the eigenvalues of the Gram matrix K as an estimation of the optimal parameter θ. Since in the definition of $\hat{t}_o$ the constant $C(\rho, D, M, M_K, \nu, \theta, \gamma)$ is non-computable in practice, we propose considering the following stopping rule $\hat{t}$, where the threshold for the smoothed empirical risk is of the order $\mathcal{O}\left(\frac{\mathrm{tr}(K^\theta)}{n}\right) = \mathcal{O}\left(\frac{\log n}{n}\right)$. This stopping rule aims at estimating an iteration of the intersection of the smoothed bias and smoothed variance.

$$\hat{t} = \inf \left\{ t > 0 : R_{\theta,t} \leq \frac{\sigma^2}{n} \sum_{i=1}^{r} \hat{\mu}_i^\theta \left[(\gamma_i^{(t)})^2 + (1 - \gamma_i^{(t)})^2 \right] \right\}. \tag{3}$$

4 Simulations

We perform simulations experiments on a simple problem: for the regression model $y_i = f^*(x_i) + \sigma \epsilon_i$, $i = 1, \ldots, n$, where $\epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)$ and $\sigma = 0.2$, we use a fixed design setting $x_i = i/n$. We have implemented the gradient descent and kernel ridge regression algorithms with a fixed step-size and fixed parameter

α. We choose the regression function to be either a smooth function $f^*(x) = -0.5 \sin\big[3(x-2)\big]$ (SF) or a piecewise linear function $f^*(x) = |x - 0.5| - 0.5$ (WF), and the polynomial decay first-order Sobolev kernel $\mathbb{K}(x_1, x_2) = \min(x_1, x_2)$. We would like to compare our stopping rule $\hat{t}$ to the previous discrepancy principle stopping rule τ described in (2), to another stopping rule t_w [7], that provides state-of-the-art results for gradient descent and kernel ridge regression algorithms in RKHS, and is based on upper bounding the bias and variance with high probabilities, as well as to the oracle method that requires the knowledge of f^*, therefore non-computable in practice.

$$t_{\text{or}} = \inf_{t>0} \Big[\mathbb{E}_\epsilon \|F^t - F^*\|_n^2 \Big]. \tag{4}$$

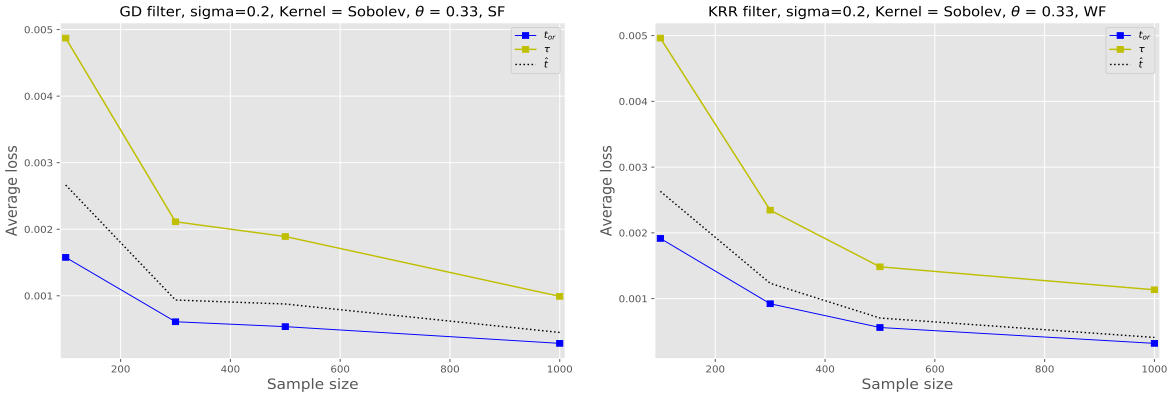

Figure 1: We choose the first-order Sobolev kernel, noise level $\sigma = 0.2$ and apply GD and KRR (linear parameterization) filters with $\alpha = 0.5$, for (SF) and (WF) regression functions. Smoothing parameter θ is chosen to be equal to the inverse of the decay of the eigenvalues of the Gram matrix. Each curve for both of two graphs corresponds to the mean-squared error of a spectral filter estimator, stopped at t_{or}, τ and $\hat{t}$, and averaged over 100 independent trials.

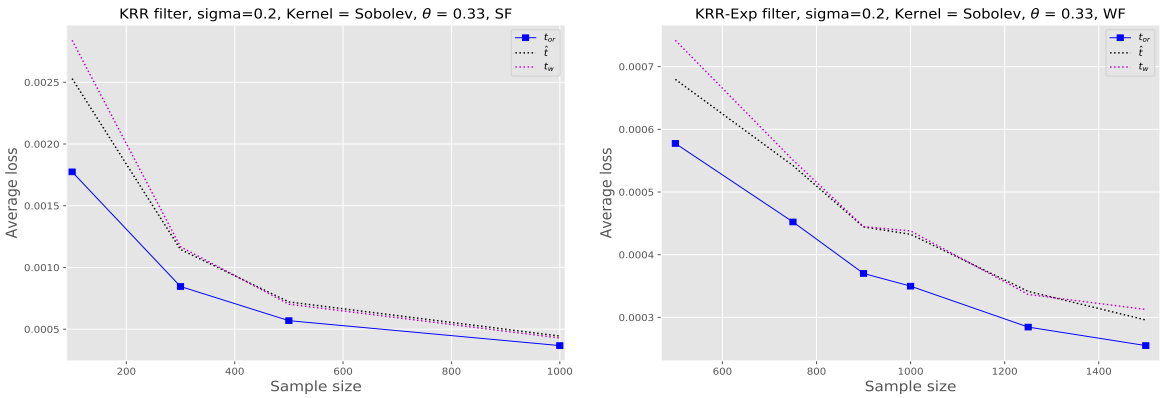

Figure 2: We choose the first-order Sobolev kernel, noise level $\sigma = 0.2$ and apply KRR (linear parameterization) and KRR (exponential parameterization) filters with $\alpha = 0.5$, for (SF) and (WF) regression functions. Smoothing parameter θ is chosen to be equal to the inverse of the decay of the eigenvalues of the Gram matrix. Each curve for both of two graphs corresponds to the mean-squared error of a spectral filter estimator, stopped at t_{or}, t_w, and $\hat{t}$, and averaged over 100 independent trials.

Figure 1 compares the resulting mean-squared errors $\|f^t - f^*\|_n^2$ of our stopping rule (3), the previous discrepancy principle rule (2) and the oracle stopping rule (4). The new proposed rule exhibits better performance than (2) for all sample sizes. Figure 2 compares the resulting mean-squared errors of our stopping rule (3), the state-of-the-art stopping rule t_w [7] and the oracle stopping rule (4). The new proposed rule exhibits better performance than t_w for the samples size $n < 300$ for the KRR (linear parameterization) filter and for the sample sizes $n < 800$ for the KRR (exponential parameterization) filter. Nevertheless, we observe the same asymptotic behaviour of t_w and $\hat{t}$. Since the rule t_w is proved to be minimax optimal in the functional space generated by the first-order Sobolev kernel, we can conclude that $\hat{t}$ recovers the same (minimax) rate in the present simulations.

5 Conclusion

In this paper we have described spectral filter algorithms (gradient descent, Tikhonov regularization) for the non-parametric regression function estimation in RKHS. We proposed a new early stopping rule $\hat{t}$ for these algorithms. After that, we proved an optimal (in terms of rate) $L_2(\mathbb{P}_X)$ out-of-sample error for the developed rule. At the end of the paper, we showed the performance of $\hat{t}$ in simulations. The main deficiency of our strategy is that the construction of $\hat{t}$ is based on the assumption that the regression function belongs to a known RKHS. Besides that, the results were derived only for the polynomial eigenvalue decay kernels.

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